LEPStats4LHC: Documentation & User Manual

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Abstract

This document describes the LEPStats4LHC package. It provides a description of the program elements, various tests and control results, and a user's manual.

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1 Introduction

This package is primarily designed to assess the discovery potential of a future experiment. The focus of this package is on hypothesis testing and not on limit setting. The package was developed for studies of the ATLAS detector's potential to discover the Standard Model Higgs Boson. During the development of this package, several technical challenges were encountered which were not relevant at the LEP experiments. This document will detail the formalism of the calculation and point out those modifications to the techniques used at LEP. Furthermore, this document will outline the layout of the software, provide a number of tests, and serve as a user's manual.¹

This package was the subject of "Challenges in Moving the LEP Higgs Statistics to the LHC" by K.S. Cranmer, B. Mellado, W. Quayle, Sau Lan Wu, which was published in the proceedings of PhyStat2003, PSN MODT004 and available via the arxiv at [physics/0312050].

The package includes a number of useful functions as well as a number command line interfaces which calculates the significance in terms of Gaussian "sigma". There are four main components to the package:

- PoissonSig Used to calculate the signficance of a number couting analysis.
- **PoissonSig_syst** Used to calculate the significance of a number counting analysis including systematic error on the background expectation.
- **Likelihood** Used to calculate the combined significance of several search channels or to calculate the significance of a search channel with a discriminating variable.
- Likelihood_syst Used to calculaate the combined significance of several search channels including systematic errors associated with each channel.

The package also includes tools to aid in calculating the luminosity necessary to achieve the 5σ discovery threshold and contours of $-2 \ln Q$ like Figure ??.

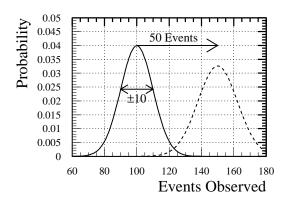
2 The Formalism

The formalism here is that which was used by the LEP Higgs working group [?, ?]: it is a classical, or *frequentist*, technique. In order to include systematic errors, the Cousins-Highland approach has been adopted [?]. Furthermore, specific numerical techniques

¹This package was previously called UWStatTools, but is no longer available via the wisconsin.cern.ch website. it is now being distributed via PhyStat.org.

used at ALEPH which perform covolutions using the Fourier Transform are utlized [?]. These techniques are by no means unique; the debate between *frequentist* and *Bayesian* methods have filled volumes [?]. These techniques are what were used for LEP Higgs searches and to that extent they have become, to some degree, accepted (or at least acceptable) to the community.

2.1 Convention to Convert CL_b to Gaussian Significance



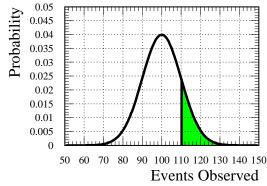


Figure 1: The left plot shows the distribution of observed events for a) the background-only hypothesis (solid line, 100 events) and the signal-plus-background hypothesis (dashed line, 150 events). The notion of Gaussian significance is illustrated by the separation of the median of the signal-plus-background distribution from the median of the background-only distribution (in units of the background-only distribution's standard deviation). The right plot shows the background-only confidence level for a signal expectation 10 events (shaded in green).

When we perform (or prepare for) a search for a new particle, we consider two hypotheses: the null hypothesis (usually referred to as the background-only hypothesis in particle physics), and some test hypothesis (usually referred to as the signal-plusbackground hypothesis in particle physics). Consider the pedagogical example of a background process that on average produces 100 background events in a detector during some time interval. If we were to repeat this exeriment many times, we would see some fluctuation in the observed number of events described by a Poisson distribution. This distribution is roughly Gaussian for large numbers of observed events. If we wanted to test for the presence of a signal in addition to the background process, then we can not state with total confidence if that signal is present or not. This is because there is some probability that the background might fluctuate to mimic the presence of a signal. To claim a discovery, the field requires a "5\u03c3" effect - a term that is related to a geometrical picture shown in Figure 1. A 5σ effect means that the background would have to fluctuate by 5 of its standard deviations above its mean in order to mimick the signal. The chance that a fluctuation this large would occur is 2.85×10^{-7} . The more fundamental concept in the 5σ discovery requirement is this probability, referred to as the background-only confidence level, CL_b .

In more general cases, the signal and background distributions are not Gaussian, though the expression of the sensitivity in terms of Gaussian significance is intuitive. It would therefore be nice to adapt this definition to a more general distribution. To

do so, first we define the background confidence level,

$$CL_b = \int_N^\infty \rho_b(n) dn \tag{1}$$

which is the probability of observing N or more events if the background-only hypothesis is true. In this equation, ρ_b is the probability density function (pdf) for observations given the background-only hypothesis. It is worth pointing out that we could use something other than the number of events to quantify the outcome of an individual experiment. In general, any test statistic which can quantify an individual experiment could replace the role of n in Equation 1 (see Section 2.2).

This background confidence level is computed on a one-sided confidence interval, meaning that the interval is bounded by N on one side, and infinity on the other. Such a quantity can be converted into an equivalent number of Gaussian standard deviations in a straightforward way. Taking a Gaussian distribution with mean 0 and standard deviation 1, find the boundary, x, of a one-sided confidence interval for which the confidence level equals the confidence level of interest. In particular, we want the value of x which satisfies

$$CL_b = \frac{1 - \operatorname{erf}(x/\sqrt{2})}{2}.$$
 (2)

where $\operatorname{erf}(x) = (2/\sqrt{\pi}) \int_x^{\infty} \exp(-y^2) dy$.

A significance of 0σ corresponds to x = 0 and a confidence level of 0.5, a significance of 1σ corresponds to x = 1 and a confidence level of (1 - 0.68)/2) = 0.16, and a significance of 5σ corresponds² to x = 5 and a confidence level of 2.85×10^{-7} .

It should further be noted that this type of generalization of significance measures distance not from the mean of the background distribution, but from the median. The transformation from number of events to confidence level and the transformation from confidence level to significance are quite non-linear. Thus the mean of the signal-plus-background distribution will be different if computed in terms of number of events, confidence level or significance. To avoid this ambiguity, using the median of the signal-plus-background curve when estimating the significance is preferable to the mean, as this provides a single, well-defined value.

2.2 The Likelihood Ratio as a Test Statistic

An efficient test statistic that can be used to combine channels is the likelihood ratio [?]. The likelihood ratio is simply the ratio of the likelihood for the signal-plus-background

²This is a purely conventional conversion from confidence level to significance. Sometimes this equivalence is quoted as 5.8×10^{-7} , but careful consideration will yield the conclusion that this is the probability of being 5 or more standard deviations *away* from the background expectation, not 5 or more standard deviations *above* the background expectation. Equation 2 is the definition consistent with the heuristic.

hypothesis to the background-only hypothesis,

$$Q = \frac{\mathcal{L}_{s+b}}{\mathcal{L}_b} = \frac{(sf_s + bf_b)}{bf_b} = 1 + \frac{sf_s}{bf_b}.$$
 (3)

In the case that the experiment is a number counting experiment, ρ_s and ρ_b are Poisson distributions and Q can be written as

$$Q = \frac{\mathcal{L}_{s+b}}{\mathcal{L}_b} = \frac{e^{-(s+b)}(s+b)^N/N!}{e^{-b}b^N/N!} = e^{-s}\left(1 + \frac{s}{b}\right)^N.$$
(4)

For convenience, the natural logarithm of this expression,

$$q = \ln Q = -s + N \ln \left(1 + \frac{s}{h} \right) \tag{5}$$

is often taken. It can immediately be seen that this expression consists of an offset (-s) and a term proportional to the number of events observed. This proportionality factor can be considered to be an event weight, though in this simple example, all events are given the same weight. Given this fact, the conversion to likelihood ratio has no impact on the significance of a simple counting analysis.

2.3 Combining Channels and the Likelihood Ratio

To combine two channels, one simply multiplies the likelihood ratios together (or adds the log-likelihood ratios). For N_{ch} channels, this becomes

$$q = \ln Q = -\sum_{i=1}^{N_{ch}} s_i + \sum_{i=1}^{N_{ch}} N_i \ln \left(1 + \frac{s_i}{b_i} \right)$$
 (6)

where s_i , b_i and N_i are the signal expectation, background expectation and number of events observed for the i^{th} channel. This can be seen to consist of an offset which is the total signal expectation for all channels and a sum over candidates, where each candidate is given a weight dependent on its channel's purity.

As in the single channel case, the confidence level can be computed using the Poisson probabilities for observing various numbers of events. With multiple channels, however, this is much more complicated, as the probability density function (pdf) for two channels is the convolution of the single channel pdf with itself.

$$\rho_{AB}(q) = \int_{-\infty}^{\infty} \rho_A(q')\rho_B(q - q')dq'. \tag{7}$$

As a result, the multi-channel probability distribution is usually computed with Monte Carlo techniques. Monte Carlo techniques, however, have the drawback that it is quite time consuming to generate a sufficiently large sample when computing significances larger than a few standard deviations and the number of expected events is quite large. Fortunately, one can make use of analytic methods, which perform the convolution via fast Fourier Transform (FFT), to compute the multi-channel probability distribution quickly and accurately [?]. This will be expounded upon in the Section 2.5.

2.4 Discriminating Variables

From a statistical point of view, calculating the likelihood with a discriminating variable is the continuous limit of combining multiple channels (see Equation 6). Just as there were channels with low and high purity, there are regions in the discriminating variable with low and high purity. In LEP Higgs searches, the discriminant variable was typically the reconstructed Higgs mass, a neural network output, or a b-tagging variable. From Monte Carlo, it is possible to construct estimates of the signal and background pdf's $f_s(x)$ and $f_b(x)$, respectively.

The description of $f_s(x)$ and $f_b(x)$ is another area of concern. While a histogram will suffice, the discontinuities in the pdf are not desirable. Furthermore, the binning of the histogram can produce quite different discriptions of the underlying pdf. These effects lead to a systematic associated with the binning. The LEP Higgs working group adopted a kernel estimation technique presented by the author [?]. Kernel estimation techniques offer an unbinned and non-parametric estimate of the pdf.

For a single event with $x = x_i$, the log-likelihood ratio generalizes in a straight forward manner,

$$q(x_i) = \ln Q(x_i) = -s + \ln \left(1 + \frac{sf_s(x_i)}{bf_b(x_i)} \right). \tag{8}$$

In this way, $f_s(x)$ and $f_b(x)$ are mapped into an expected distribution of q(x). For the background-only hypothesis, $f_b(x)$ provides the probability of corresponding values of q needed to define the single event pdf ρ_1 .

$$\rho_{1,b}(q(x)) = f_b(x) \tag{9}$$

The construction of the ρ_1 distributions for signal and background is typically obtained by scanning over the discriminating variable x. The result of this discrete scan is that the continuous f(x) is not mapped into a continuous ρ_1 distribution. This is an area for improvement. Because the map from $q(x): x \to q$ is many-to-one, it is not invertable; thus it is difficult to interpolate. For example, samples x_i and x_{i+1} correspond to q_i and q_{i+1} such that $\rho_1(q_i) = f(x_i)$ and $\rho_1(q_{i+1}) = f(x_{i+1})$, but for $q^* \in [q_i, q_{i+1}]$ it is not clear what $\rho_1(q^*)$ is because we do not have the (possibly many) corresponding $f(x^*)$. One possibility is to use kernel estimation on the samples q_i with weights $\rho_1(q_i)$ to produce a continuous estimate of ρ_1 distribution [?]. This technique is only applicable for the case of a discriminating variable and should not be used for a naturally discrete combination of multiple channels. The bare essentials for this technique are included in the code, see Section 3.1.2.

2.5 The Fourier Transform Technique

For multiple events, the distribution of the log-likelihood ratio must be obtained from repeated convolutions of the single event distribution [?]. In the Fourier domain, denoted with a bar, the distribution of the log-likelihood for n particles is

$$\overline{\rho_n} = \overline{\rho_1}^n \tag{10}$$

Thus the expected log-likelihood distribution for background takes the form

$$\rho_b(q) = \sum_{n=0}^{\infty} \frac{e^{-b}b^n}{n!} \rho_{n,b}(q)$$
(11)

which in the Fourier domain is simply

$$\overline{\rho_b(q)} = e^{b[\overline{\rho_{1,b}(q)} - 1]}. (12)$$

For the signal-plus-background hypothesis we expect s events from the $\rho_{1,s}$ distribution and b events from the $\rho_{1,b}$ distribution which leads to

$$\rho_{s+b}(q) = \sum_{n=0}^{\infty} \frac{e^{-b}b^n}{n!} \rho_{n,b}(q) + \sum_{n=0}^{\infty} \frac{e^{-s}s^n}{n!} \rho_{n,s}(q).$$
 (13)

In the Fourier domain ρ_{s+b} is simply

$$\overline{\rho_{s+b}(q)} = e^{b[\overline{\rho_{1,b}(q)} - 1] + s[\overline{\rho_{1,s}(q)} - 1]}.$$
(14)

Perhaps it is worth noting that $\overline{\rho(q)}$ is actually a complex valued function of the Fourier conjugate variable of q. Thus numerically the exponentiation in Equation 14 requires Euler's formula $e^{i\theta} = \cos \theta + i \sin \theta^3$.

Numerically these computations are carried out with the Fast Fourier Transform (FFT). The FFT is performed on a finite and discrete array, beyond which the function is considered to be periodic. Thus the range of the ρ_1 distributions must be sufficiently large to hold the resulting ρ_b and ρ_{s+b} distributions. If they are not, the "spill over" beyond the maximum log-likelihood ratio q_{max} will "wrap around" leading to unphysical ρ distributions. Because the range of ρ_b is much larger than $\rho_{1,b}$ it requires a very large number of samples to describe both distributions simultaneously. This subject is taken up in more detail in Section 3.1. The nature of the FFT results in a number of round-off errors and limit the numerical precision to about 10^{-16} – which are significant for consistently describing the significance beyond about 8σ . Extrapolation techniques and Arbitrary Precision calculations can overcome these difficulties and are the subject of Sections 2.8 and 2.9, respectively.

³Can't resist pointing out $e^{i\pi} + 1 = 0$

2.6 Systematic Uncertainty & Correlated Systematic Uncertainty

For signal and background composed of several different processes, it is possible to simply add the processes together to form a total signal and background contribution. Thus far we have simplified the calculation by implicitly using $s = \sum_{i}^{N} s_i$ and $b = \sum_{j}^{M} b_j$ where s_i is the number of signal events in the i^{th} process and b_j is the number of background events in the j^{th} process. It would also be possible to establish a ρ_1 distribution for each process and, for instance, write

$$\overline{\rho_b}(q) = e^{\sum_j^M n_j [\overline{\rho_{1,j}(q)} - 1]}.$$
(15)

If we consider systematic uncertainty on the number of events n_i expected for the i^{th} process, then it is advantageous to write the distributions this way. This form allows each process to have its own systematic uncertainty and even for a correlated systematic error matrix S_{ij} .

$$S_{ij} = \langle (n_i - \langle n_i \rangle)(n_j - \langle n_j \rangle) \rangle \tag{16}$$

The Cousins-Highland formalism for including systematic errors on the normalization of the signal and background is provided in [?] and generalized in [?, ?]. The method considers an ensemble of possible values of the unkown n_i weighted by a Gaussain probability based on S_{ij} ⁴.

$$\overline{\rho_{sys}(q)} = \int \dots \int e^{\sum_{i}^{K} n_{i} [\overline{\rho_{1,i}(q)} - 1]} \left(\frac{1}{\sqrt{2\pi}}\right)^{K} \frac{1}{\sqrt{|S|}}$$

$$e^{\sum_{i}^{K} \sum_{j}^{K} - \frac{1}{2} (n_{i} - \langle n_{i} \rangle) S_{ij}^{-1} (n_{j} - \langle n_{j} \rangle)} \prod_{i} dn_{i}$$
(17)

Reference [?] provides a analytic expression for the log-likelihood ratio distribution including a correlated error matrix; however, that equation was obtained with an integration over negative numbers of expected events and does not hold. Attempts to provide a closed form for the positive semi-definite region require analytical continuation of the error function over a wide range of the complex plane. Instead, a numerical integration over the positive semi-definite region has been adopted. The various integration techniques are the subject of Section 3.2.

The fact that negative n_i occur in Equation 17 is enough to show that the distribution of n_i is not strictly Gaussian. In principal any distribution could be used within this framework. Internal consistancy of this method requires that one can parametrize this disbribution of n_i to at least the same precision as the confidence level they wish to explore. I.e. to claim a $x\sigma$ discovery, one must know the systematic error associated with the background hypothesis to the $x\sigma$ level. This is a very difficult task experimentally and raises a number of the more philosophical debates in the statistics world.

⁴Technically this is not a convolution because, while, the Gaussian kernel is fixed, the ρ distributions depend on n_i the domain of the "convolution".

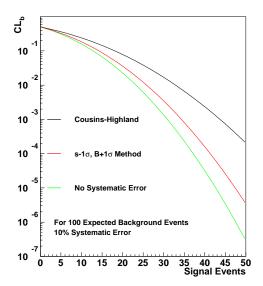


Figure 2: Comparison of CL_b for Cousins-Highland and $s-1\sigma$, $b+1\sigma$ methods.

If we take the systematic uncertainty on n_i to be some fixed fraction δ of n_i (e.g. a 10% systematic uncertainty), and we impose that we do not have any negative values of n_i then we arrive at a maximum significance $x\sigma$ which we can explore in an internally consistent way:

$$x < 1/\delta. \tag{18}$$

There are variations on this method in which Gaussian systematic errors are truncated beyond some number of standard deviations. These may well be better discriptions of the true uncertainty in n_i than an unrestricted Gaussian. Another method which is somewhat common is to incorporate systematic uncertainty in a reasonable and pessimistic way. The method consists of simply reducing the number of signal events expected by 1σ and increasing the number of background events expected by 1σ . It does not rely on an ensemble of possible values of n_i , but instead a particular and pessimistic scenario. Without going into the relative merits of these two methods, consider a simple number counting analysis with an expected background of 100 events and a 10%systematic uncertainty in this expectation. For a 100 events the Poisson distribution can be well approximated by a Gaussian distribution (and this will ease the calculation and the example). In the Cousins-Highland formalism we can approximate Equation 17 as a convolution of two Gaussians (each with standard deviation 10 events) which results in another Gaussian centered at 100 with a standard deviation of $10\sqrt{2} \approx 14.14$ events. Due to the bounds placed by Equation 18 we can reliably explore CL_b up to about the 10σ level, so we will consider a signal expectation from 0 to 50 events $(0-5\sigma)$. For a Gaussian background distribution the CL_b is a simple expression with the error function. In Figure 2 we compare these two methods and see that the Cousins Highland produces a higher CL_b (lower significance) than the $s-1\sigma$, $b+1\sigma$ method.

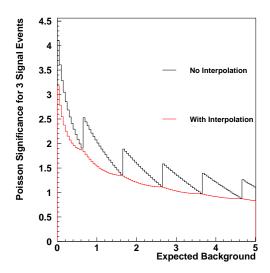


Figure 3: The pathological behavior of the unmodified Poisson significance calculation (black). It is not only discontinuous, but also increases as the background expectation increases. Continuity is restored with interpolation (red).

2.7 Interpolation

In a number counting experiment the background confidence level calculation for an observation will be based on an integer-valued observed number of events N and a real-valued expected number of events b. In this case the CL_b will be given by

$$CL_b = \sum_{i=N}^{\infty} P(i;b) = \sum_{i=N}^{\infty} e^{-b} b^i / i!.$$
 (19)

However, when assessing the discovery potential for a future experiment, we may expect a real-valued number of observed events. Initially, the PoissonSig program was written such that it would find the median of the Poisson distribution associated with the signal-plus-background distribution (an integer) and then use that as N in the equation above. This leads to the pathological behavior seen in Figure 3: the significance is not only discontinuous, but also increases as the background expectation increases. Let us consider the behaviour for 3 signal events in the case of 4.64 and 4.7 background events. Figure 4 shows the cumulative distribution of the signal-plus-background distribution is hardly changed between these two points; however, the median changes discontinuously due to the discreteness of the Poisson distribution. Thus for 4.65 background events N=6 and for 4.7 background events N=7. Thus for 4.7 background events the CL_b is less (the significance is higher).

By simply interpolating the cumulative probability and finding its intersection with 1/2, we can produce a generalized median that changes continuously. With the gen-

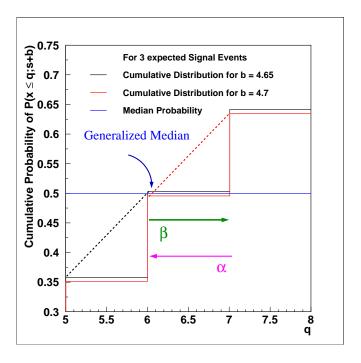


Figure 4: Discontinuous change in the Median of the signal-plus-background distribution. Diagram of the Generalized Median.

eralized median of the signal-plus-background distribution we wish to evaluate CL_b . Because the Poisson distribution is discrete, we must also generalize the CL_b calculation. This is done as follows:

- Let x_0 be the last integer with $P(x \le x_0; s + b) < 1/2$.
- Linearly Between Interpolate $x_0 \& x_0 + 1$ to find $\beta \& \alpha$.
- Generalize the median as $\tilde{\mu} = x_0 + \beta$.
- Generalize CL_b as $P(x \geq \tilde{x}; b) := \alpha P(x \geq x_0; b) + \beta P(x \geq x_0 + 1; b)$

The same situation occurs in the case of the a likelihood ratio calculation, however; the values of the likelihood ratio need not be integer-valued. Computationally, the ρ_{s+b} distribution is a histogram possibly with many empty bins between the adjacent non-empty bins q_0 and q_1 . Thus one must slightly modify the interpolation algorithm above such that $\alpha, \beta \in [0, 1], x_0 \to q_0$ and $x_0 + 1 \to q_1$.

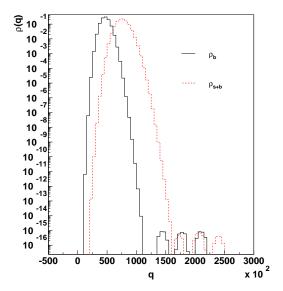


Figure 5: Illustration of the numerical "noise" which appears for $\rho(q) \lesssim 10^{-16}$.

2.8 Extrapolation

The numerical limitations in the Fourier Transform Technique (introduced in Section 2.5) are the result of many round-off errors in the FFT. Figure 5 illustrates a representative ρ_b and ρ_{s+b} distributions spanning over 16 orders of magnitude. It is apparent that the the numerical precision is a limitation when the median of the signal-plus-background distribution is located in these unreliable regions. For double precision floating point numbers, these effects limit the ability to calculate significances above about 8σ . In Section 2.9 we discuss a solution to this problem in which the FFT is implemented with an arbitrary precision library; however, this method is excruciatingly slow and memory intensive. Thus, in this section various extrapolation techniques are described.

The first extrapolation technique to be applied was a simple "Gaussian extrapolation" in which the ρ_b distribution was described by a Gaussian with the same mean μ_b and standard deviation σ_b (not really a fit in the common sense of the word). In this case the significance was simply quoted as $\sigma = (\tilde{\mu} - \mu_b)/\sigma_b$ (see Figure 6). For calculations with many events, the Gaussian approximation is expected to be valid. Because the Gaussian distribution allows for $\rho_b(q < -s_{tot}) > 0$ we expect the Gaussian extrapolation technique to overestimate the significance in general. This behavior can be seen in Figure 7.

The second method we studied was based on a Poisson fit to the ρ_b distribution. The Poisson distribution has the desirable properties that it will have no probability below the hard limit and that its shape is more appropriate. However, the Poisson distribution is a discrete distribution thus we must find some affine transformation

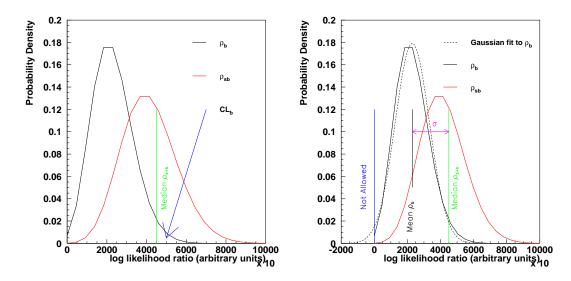


Figure 6: Diagram for the Gaussian extrapolation technique. The abcissa corresponds to the histogram bin index of the log-likelhood ratio, in which the 0^{th} bin corresponds to the lower limit $q = -s_{tot}$ (see Equation 5).

between the space of the log-likelihood ratio and the space of the Poisson distribution. This is accomplished as follows: First we use the identity that for a Poisson distribution the $P(x;\mu)$ the mean is given by μ and the variance is given by μ . Next we assume that our distribution $\rho_b(q)$ takes the form of a Poisson with $q = \alpha x$, which forces $\text{mean}(\rho_b) = \alpha \mu$ and $\text{var}(\rho_b) = \alpha^2 \mu$. This gives us two equations which we can use to solve for μ and α . With those parameters, the median of the signal-plus-background distribution and the mean of the background-only distribution can be transformed via α to produce the corresponding Poisson significance.

Figure 7 offers a comparison of these methods for an example ATLAS Higgs combined significance calculation. For reference a (green-dotted) curve obtained from adding in quadrature (green dotted line) is included. The red dashed line corresponds to the unmodified likelihood ratio which can not produce significance values above about 8σ . The Gaussian extrapolation technique tends to overestimate the significance, while the Poisson extrapolation is well behaved across the entire mass range. The VBF channels and the channels discussed in [?] are used for this combination. This figure is meant to demonstrate the different methods of combination and does not include updated numbers for non-VBF analyses. No systematic errors on background normalization have been included.

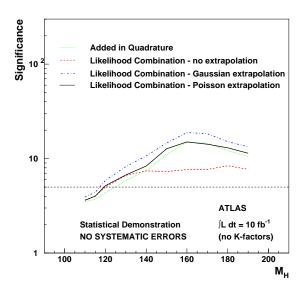


Figure 7: Comparison of the combined significance obtained from adding in quadrature (green dotted line) and various likelihood ratio combinations. The red dashed line corresponds to the unmodified likelihood ratio which can not produce significance values above about 8σ (see text). To solve this problem Gaussian (blue dash-dotted line) and Poisson (black solid line) extrapolation techniques have been developed.

2.9 Accessing Low CL_b with Arbitrary Precision Libraries

This has not yet been implemented in this code, but has in another package. The CLN libraries handel arbitrary precision numbers with which an arbitrary precision FFT can be implemented. This allows one to calculate CL_b to arbitrary low levels.

3 The Implementation

The LEPStats4LHC package contains the code for three libraries and a number of sample programs. The Library is broken down into conceptual elements. The Poisson and Likelihood calculations are, for the most part, idependent from each other because the ρ distributions have different test statistics for their domain. The integration, median, and interpolation calculations are largely unified into a set of common tools.

3.1 Binning the Likelihood Ratio Distributions

3.1.1 MAX_SIGMA global definition

3.1.2 The sampleLR Function

3.1.3 The getMaxLogLR Function

```
double getMaxLogLR(double* sig, double* back, int nbins) {
 double max = 0;
 double totalsb = 0, totalb = 0;
 double LR, temp, factor = 0, maxSysError = 0.1, maxSigma = MAX_SIGMA;
 //This subroutine is to estimate how wide the log(LR) distribution
  //will be after the series of n_particle convolutions are applied.
 //The idea is that for an expected n events, the one particle LR
  //distribution will be shifted by a factor of n. From Poisson
 //statistics we expect most of the Poisson probability is around s+b
 //+/- sqrt(s+b). We leave maxSigma standard deviations for breating
 //room. So at most we expect s+b + maxSigma*sqrt(s+b) convolutions.
 //In addition, if there is systematic error, then the mean may be
  //s+b + maxSigma*maxSysError*(s+b). That's the origin of "factor"
  //Also, if there is systematic Error in the normalization, an upper
  //limit is taken into account (currently 20%).
 fprintf(stderr, "Estimating max log(LR) after convolution\n");
 for(int j=0; j<nbins; j++){</pre>
    totalsb += sig[j] + back[j];
    totalb += back[j];
 for(int j=0; j<nbins; j++){
  if(back[j] > 0){
      LR=log((sig[j]+back[j])/back[j]);
      factor = (sig[j]+back[j])*(1+maxSysError*maxSigma)
        + maxSigma*sqrt((sig[j]+back[j]));
        max += LR*factor;
 }
 return max;
```

3.2 Various Ways To Incorporate Systematic Errors

4 User Manual

4.1 Instalation

The LEPStats4LHC package currently consists of three libraries with different dependencies:

- libcommontools Only requires standard C++ libraries
- **libffttools** Requires the FFTW libraries to be installed. These libraries can be obtained at: http://www.fftw.org/
- **libgsltools** Requires the FFTW libraries and the GNU Scientific Libraries (GSL). GSL can be obtained at: http://www.gnu.org/software/gsl/gsl.html

There are four important calculations which have been implemented via a simple program interfaced to these libraries. Hopefully these programs will be not only useful in their own right, but also serve as examples interfaces to the libraries. The programs and their dependencies are:

- **PoissonSig** Used to calculate the signficance of a number couting analysis. Depends on libcommontools and TestPoissonSig.cc.
- PoissonSig_syst Used to calculate the significance of a number counting analysis including systematic error on the background expectation. Depends on libcommontools and TestPoissonSig_syst.cc.
- Likelihood Used to calculate the combined significance of several search channels or to calculate the significance of a search channel with a discriminating variable. Depends on libcommontools, libffttools and TestLikelihood.cc.
- Likelihood_syst Used to calculate the combined significance of several search channels or to calculate the significance including systematic errors associated with each channel. Depends on libcommontools, libffttools, libgsltools and TestLikelihood_syst.cc.

The GNU Makefile organizes the various source files into the three different libraries. So far there is no more sophisticated technique using configure.

The installation of FFTW is fairly straightforward and well documented at http://www.fftw.org/. No sophisticated settings are required for the LEPStats4LHC libraries to compile. If you do not have the ability to install FFTW as root, then you may need to change the Makefile accordingly.

The installation of GSL is also straightforward, with one exception. GSL provides a very thorough set of tests which should be run, because with gcc version 2.96 there

can be problems in the EigenSystem code when optimization is turned on. This can be overcome by simply replacing the "make" step with "make CFLAGS="-g". In the current version of LEPStats4LHC, the EigenSystem routines are not used, however, use of these routines is anticipated in forthcoming releases. Below is the expected output of the make command for LEPStats4LHC when FFTW and GSL are properly installed.

```
[cranmer@pcuw30 LEPStats4LHC]$ make
make[1]: Entering directory '/home/cranmer/LEPStats4LHC'
gcc -03 -c -o CommonTools.o CommonTools.cc
gcc -03 -c -o Interpolation.o Interpolation.cc
gcc -03 -c -o Kernel.o Kernel.cc
gcc -03 -c -o PDE.o PDE.cc
gcc -03 -c -o TestStatistic.o TestStatistic.cc
gcc -03 -c -o PoissonSig.o PoissonSig.cc
gcc -03 -c -o PoissonSig_syst.o PoissonSig_syst.cc
gcc -03 -c -o FFT_Tools.o FFT_Tools.cc
gcc -03 -c -o Convolution.o Convolution.cc
gcc -03 -c -o Extrapolation.o Extrapolation.cc
gcc -03 -c -o Likelihood.o Likelihood.cc
gcc -03 -c -o ErrorMatrix.o ErrorMatrix.cc
gcc -03 -c -o CousinsHighland.o CousinsHighland.cc
gcc -03 -c -o Likelihood_syst.o Likelihood_syst.cc
ar rcv libcommontools.a CommonTools.o Interpolation.o Kernel.o PDE.o TestStatistic.o PoissonSig.o PoissonSig_syst
r - CommonTools.o
r - Interpolation.o
r - Kernel.o
r - PDE.o
r - TestStatistic.o
r - PoissonSig.o
r - PoissonSig_syst.o
ranlib libcommontools.a
ar rcv libffttools.a FFT_Tools.o Convolution.o Extrapolation.o Likelihood.o
r - FFT_Tools.o
r - Convolution.o
r - Extrapolation.o
r - Likelihood.o
ranlib libffttools.a
ar rcv libgsltools.a ErrorMatrix.o CousinsHighland.o Likelihood_syst.o
r - ErrorMatrix.o
r - CousinsHighland.o
r - Likelihood_syst.o
ranlib libgsltools.a
make[1]: Leaving directory '/home/cranmer/LEPStats4LHC'
gcc -03 -o PoissonSig TestPoissonSig.cc \
libcommontools.a -lm
gcc -03 -o PoissonSig_syst TestPoissonSig_syst.cc \
libcommontools.a -lm
gcc -03 -o Likelihood TestLikelihood.cc \
libffttools.a libcommontools.a -lrfftw -lfftw -lm
gcc -03 -o Likelihood_syst TestLikelihood_syst.cc
libgsltools.a libffttools.a libcommontools.a \
-lrfftw -lfftw -lm -lgsl -lgslcblas
gcc -03 -o TestErrorMatrix TestErrorMatrix.cc \
libgsltools.a -lm
                   -lgsl -lgslcblas
```

Below is a snapshot of the files included in the release.

```
[cranmer@pcuw30 LEPStats4LHC]$ ls -ltr
total 168
                                   568 May 5 13:40 PDE.h
-rw-r--r--
            1 cranmer zp
          1 cranmer zp
-rw-r--r--
                                  3297 May 5 13:40 PDE.cc
          1 cranmer zp
-rw-r--r--
                                   813 May 5 13:40 Kernel.h
            1 cranmer zp
-rw-r--r--
                                  1243 May 5 13:40 Kernel.cc
-rw-r--r--
            1 cranmer zp
                                   160 May 5 15:29 Convolution.h
           1 cranmer zp
-rw-r--r--
                                   184 May 5 15:31 Extrapolation.h
-rw-r--r--
                                  212 May 5 15:33 PoissonSig.h
           1 cranmer zp
            1 cranmer zp
-rw-r--r--
                                   297 May 5 16:09 ErrorMatrix.h
-rw-r--r--
            1 cranmer zp
                                   657 May 5 16:16 CousinsHighland.h
-rw-r--r 1 cranmer zp
                                  967 May 5 16:44 PackageLayout.txt
-rw-r--r-- 1 cranmer zp
                                2428 May 5 17:42 TestErrorMatrix.cc
          1 cranmer zp
-rw-r--r--
                                   905 May 6 17:15 Likelihood.h
            1 cranmer zp
                                  1659 May 6 17:22 ErrorMatrix.cc
-rw-r--r--
-rw-r--r--
            1 cranmer zp
                                  1233 May 6 17:24 Convolution.cc
           1 cranmer zp
                                 1845 May 6 17:25 DiscoveryPlot.cc
-rw-r--r--
-rw-r--r--
           1 cranmer zp
                                 1786 May 6 17:25 Extrapolation.cc
                                 2322 May 6 17:26 TestGSL.cc
-rw-r--r--
           1 cranmer zp
-rw-r--r--
                                   949 May 6 17:28 TestLikelihood.cc
            1 cranmer zp
-rw-r--r--
                                 1246 May 6 17:28 TestLikelihood_syst.cc
            1 cranmer zp
-rw-r--r- 1 cranmer zp
                                  365 May 6 17:28 TestPoissonSig.cc
-rw-r--r-- 1 cranmer zp
                                   479 May 6 17:29 TestPoissonSig_syst.cc
                                   287 May 7 14:08 FFT_Tools.h
-rw-r--r--
           1 cranmer zp
                                  1479 May 7 14:17 FFT_Tools.cc
-rw-r--r--
            1 cranmer zp
-rw-r--r--
            1 cranmer zp
                                 12673 May 7 14:21 Likelihood_syst.cc
           1 cranmer zp
                                  2191 May 7 14:27 TestStatistic.cc
-rw-r--r--
           1 cranmer zp
-rw-r--r--
                                   458 May 7 14:28 TestStatistic.h
4091 May
                                           7 14:54 PoissonSig.cc
                                           7 15:02 Likelihood.cc
                                  9650 May
-rw-r--r 1 cranmer zp
                                   488 May 7 15:06 Interpolation.h
-rw-r--r-- 1 cranmer zp
                                   283 May 7 15:06 CommonTools.h
          1 cranmer zp
-rw-r--r--
                                  2654 May 7 15:06 CommonTools.cc
          1 cranmer zp
-rw-r--r--
                                  3155 May 7 15:07 Interpolation.cc
-rw-r--r--
                                  7914 May
                                           7 15:20 CousinsHighland.cc
            1 cranmer zp
            1 cranmer zp
-rw-r--r--
                                  3504 May 7 15:23 PoissonSig_syst.cc
-rw-r--r-- 1 cranmer zp
                                  1561 May 7 15:28 Makefile
                                  1621 May 7 15:49 README
-rw-r--r--
           1 cranmer zp
```

4.2 Program Usage

The use of the example programs is very simple. For an experiment with S expected signal events and B expected background events, the Poisson Significance is given by:

PoissonSig
$$S\ B$$

If one wishes to include a relative uncertainty Δ in the background (e.g. $\Delta = 0.1$ for a 10% relative uncertainty), the Poisson Significance is given by:

PoissonSig_syst
$$S$$
 B Δ

If one wishes to combine k channels or, equivalently, to include a discriminating variable with k histogram bins, the significance using the Likelihood ratio as a test statistic is given by:

Likelihood
$$S_1 \ldots S_k B_1 \ldots B_k$$

If one wishes to combine k channels each with a background uncertainty of Δ_i the significance using the Likelihood ratio as a test statistic is given by:

Likelihood_syst
$$S_1$$
 ... S_k B_1 ... B_k Δ_1 ... Δ_k

If one wishes to consider an experiment with a discriminating variable and a systematic error on the overall normalization of the background, then slight changes need to be made to TestLikelihood_syst.cc. Similarly, if one wishes to include several different processes which together comprise the signal or background expectations and consider (possibly correlated) uncertainties on each process, then more significant changes need to be made to TestLikelihood_syst.cc. These changes will be discussed in Secton 4.4. See Section 5 for examples and "control results" with wich a new user can check their code is running properly.

4.3 Output to stdout & stderr

In general the output of the programs is directed to two different streams: stdout and stderr. In order to ease the use of the above programs with scripting languages, only the resulting significance (without a following carrage return) is sent to stdout. The rest of the output messages are directed to stderr and can be seen at the terminal.

If one wishes to direct the output of the calculation (i.e. stdout) to a file, simply:

PoissonSig
$$S$$
 B > filename

If one wishes to direct the messages (i.e. stderr) to a file, simply:

PoissonSig
$$S$$
 B 2> filename

If one wishes to direct all the output (i.e. stdout and stderr) to a file, simply

PoissonSig
$$S$$
 B > filename 2>&1

4.4 Advanced Usage

5 Tests & Control Results

In this section we present a few test cases which can also serve as "control results" with which a new user can compare. In order to compare these results with some expectation from first-principles, consider two samples with different purity and enough events that the Gaussian approximation s/\sqrt{b} is fairly good indication of the significance. The first channel (channel **a**) will have 10 expected signal and 100 expected background events. The second channel (channel **b**) will have 300 expected signal and 10000 expected background events. In both channels, the Poisson background-only distribution can be fairly well approximated by a Gaussian with standard deviation of stdev_b = \sqrt{b} . So we expect for channel **a** about 1σ and for channel **b** about 3σ . Below we see the Poisson Significance from PoissonSig.

It may seem surprising that for channel **a** that the significance is some 12% below the expectation of 1σ . This underscores the importance of the interpolation. In fact, by raising the background expectation to 100.6, the Poisson Significance without interpolation drops to 0.891117σ . Then raising it further to 100.7, the significance discontinuously jumps up to 0.977725σ . The interpolated significance, in contrast, changes continuously. For channel **b**, where the Gaussian approximation is more valid, we see almost exactly the expected 3σ .

Now we consider the incorporation of systematic errors with the Cousins-Highland formalism. Again, if we approximate the background-only distribution with a Gaussian, we can do this calculation on paper. First we point out that a convolution of two Gaussians is also a Gaussian and the standard deviation of the result is given by the sum in quadrature of the constituent Gaussians. Thus for channel **a** with 10% systematic error on the background normalization translates to an absolute systematic error of 10 events. The inherent Poissonian width of 100 events is also 10 events. Thus, the resulting standard deviation is $10\sqrt{2} = \sqrt{10^2 + 10^2} \approx 14.14$ events. Thus the significance is expected to be about 0.70721358σ . Again we see that without interpolation that the significance is close to what we expected, but when we interpolate we find the significance is about 12% lower. Indeed, if we vary the background expectation from 100.8 to 100.9 events we see the significance without interpolation discontinuously jumps from 0.625840σ up to 0.686731σ while the interplated result varies continuously.

For channel **b** a 1% systematic error translates to 100 events. Similarly the inherent Poissonian width is about 100 events. Thus the resulting standard deviation is about $100\sqrt{2} \approx 141.4$ events and we expect the significance to be about 2.1213203σ . Below we see the results from PoissonSig_syst – which are quite close to the expectation from the approximate methods above.

For a single channel the Likelihood ratio should reproduce the Poisson calculation exactly (and so should the Poisson Extrapolation technique). Below we see the results for channel **a** are reproduced with the Likelihood program.

```
[cranmer@pcuw30 LEPStats4LHC]$ ./Likelihood 10 100
------Setup Binning------
For a single Channel:
                      min log(LR) = 0.095310 max log(LR) = 0.095310
                      totalS = 10.000000 totalB = 100.000000
Estimating max log(LR) after convolution:
       bin 0: log(LR) = 0.095310, rho_b = 100.000000, rho_sb = 110.000000
Set Global log(LR): min = 0.000000 max = 26.868388 Need at least 2^9 bins, Perfect binning needs 2^9 bins
Have 2^18 bins, bins for Rho1 = 929.902881
-----Doing FFT's-----
                              = 0.000000
Problem Index for Rho_b
Problem Index for Rho_s+b
                             = 0.000000
-----About to Calculate Significance-----
Gaussian Approx: median of rho_b is 10.000108 stdev from hard limit
                Significance is 0.999892
Poisson Approx: mean of rho_b = 92900.000000, stdev = 9290.000000
                Calculated nu = 100.000000, alpha = 929.000000
                Corresponds to Poisson with b=100.000000 and s+b=109.333602
                With No interpolation: median of rho_sb = 110
                       CL_b = 1.705599e-01, Significance = 0.951955
                With interpolation: median of rho_sb = 109.333602
                       CL_b = 1.877295e-01, Significance = 0.886294
CL_b integration with no interpolation:
                median of rho_b = 102190, Significance = 0.951955
CL_b integration with interpolation:
                lowerBin = 101261, upperBin = 102190
                beta = 0.333602, generalized median = 101570.916684
                Significance with Interpolation = 0.886294
   -----Summary-----
Sigma(CL_b)
                Sigma(CL_b)(no interp)
                                              Sigma_Gauss
                                                             Sigma_Poisson
0.886294
               0.951955
                                                             0.886294
                                              0.999892
       Will use integrated CL_b because Gaussian Approx = 0.999892 < 6
Significance = 0.886294
```

We also wish to see if the calculation with systematic errors agrees. Because the Cousins-Highland formalism is implemented (in this case) with a Monte Carlo integration over the expected number of background events, the result has a relative uncertainty of about $1/\sqrt{N}$, where N is the number of Monte Carlo samples in the integration. For N=1000, this relative uncertainty is about 3.16%, which translates into an absolute uncertainty of about 0.067σ . The PoissonSig_syst and Likelihood_syst calculations agree within this margin of error.

```
[cranmer@pcuw30 LEPStats4LHC]$ ./Likelihood_syst 300 10000 .01
 ------Using the Following Uncertainty------
For Process 0: signal uncertainty = 0.000000
For Process 0: background uncertainty = 0.010000
------Setup Binning-----
For a single Channel: min log(LR) = 0.029559 max log(LR) = 0.029559
                      totalS = 300.000000
                                             totalB = 10000.000000
Estimating max log(LR) after convolution:
       bin 0: log(LR) = 0.029559, rho_b = 10000.000000, rho_sb = 10300.000000
Set Global log(LR): min = 0.000000 max = 572.019320
Need at least 2^15 bins, Perfect binning needs 2^15 bins
Have 2^18 bins, bins for Rho1 = 13.546155
-----Doing FFT's-----
 doing 1000 out of 1000 MC samples, total weight = 1.000000
totalWeight = 1.000000
 doing 1000 out of 1000 MC samples, total weight = 1.000000
totalWeight = 1.000000
                             = 0.000000
Problem Index for Rho_b
Problem Index for Rho_s+b
                             = -0.000000
-----About to Calculate Significance-----
Gaussian Approx: median of rho_b is 71.979558 stdev from hard limit
                Significance is 2.122190
Poisson Approx: mean of rho_b = 130027.773098, stdev = 1806.624032
                Calculated nu = 5180.082583, alpha = 25.101487
                Corresponds to Poisson with b=5180.082583 and s+b=5333.309402
                With No interpolation: median of rho_sb = 5334
                       CL_b = 1.685543e-02, Significance = 2.123513
                With interpolation: median of rho_sb = 5333.309402
                       CL_b = 1.725899e-02, Significance = 2.113968
CL_b integration with no interpolation:
               median of rho_b = 133874, Significance = 2.134195
CL_b integration with interpolation:
                lowerBin = 133861, upperBin = 133874
                beta = 0.999540, generalized median = 133873.994025
                Significance with Interpolation = 2.134192
-----Summary-----
Sigma(CL_b)
               Sigma(CL_b)(no interp)
                                             Sigma_Gauss
                                                            Sigma_Poisson
                                                            2.113968
2.134192
               2.134195
                                             2.122190
       Will use integrated CL_b because Gaussian Approx = 2.122190 < 6
Confidence Level is = 2.134192
```

The next thing to check is the combined significance of channels **a** and **b**. The corresponding Gaussian approximation is to add the individual channels significance in quadrature. Thus the combined significance for channels **a** and **b** without systematic error is $\sqrt{1^2 + 3^2} \approx 3.1622777\sigma$ which is in good agreement with the calculation using Likelihood.

```
[cranmer@pcuw30 LEPStats4LHC]$ ./Likelihood 10 300 100 10000
------Setup Binning-----
For a single Channel: \min \log(LR) = 0.029559 \max \log(LR) = 0.095310
                      totalS = 310.000000
                                             totalB = 10100.000000
Estimating max log(LR) after convolution:
       bin 0: log(LR) = 0.095310, rho_b = 100.000000, rho_sb = 110.000000
       bin 1: log(LR) = 0.029559, rho_b = 10000.000000, rho_sb = 10300.000000
Set Global log(LR): min = 0.000000 max = 598.887708
Need at least 2^13 bins, Perfect binning needs 2^14 bins
Have 2^18 bins, bins for Rho1 = 28.780569
-----Doing FFT's-----
                             = 0.000000
Problem Index for Rho b
Problem Index for Rho_s+b
                             = 0.000000
-----About to Calculate Significance-----
Gaussian Approx: median of rho_b is 97.860686 stdev from hard limit
                Significance is 3.161401
Poisson Approx: mean of rho_b = 124100.000000, stdev = 1268.108829
                Calculated nu = 9577.022560, alpha = 12.958098
                Corresponds to Poisson with b=9577.022560 and s+b=9886.247273
                With No interpolation: median of rho_sb = 9887
                       CL_b = 8.240269e-04, Significance = 3.147265
                With interpolation: median of rho_sb = 9886.247273
                       CL_b = 8.458213e-04, Significance = 3.139625
CL_b integration with no interpolation:
                median of rho_b = 128107, Significance = 3.141913
CL_b integration with interpolation:
                lowerBin = 128106, upperBin = 128107
                beta = 0.964233, generalized median = 128106.964233
               Significance with Interpolation = 3.141885
   -----Summary-----
Sigma(CL_b)
               Sigma(CL_b)(no interp)
                                                            Sigma_Poisson
                                             Sigma_Gauss
3.141885
               3.141913
                                             3.161401
       Will use integrated CL_b because Gaussian Approx = 3.161401 < 6
Significance = 3.141885
```

The last thing to check is the combined significance of channels **a** and **b** with systematic errors. Again we use the corresponding Gaussian approximation, and add the individual channels significance in quadrature. Thus the combined significance for channels **a** and **b** with systematic error is $\sqrt{0.70721358^2 + 2.1213203^2} \approx 2.2361018\sigma$ which is in good agreement with the calculation using Likelihood_syst.

```
[cranmer@pcuw30 LEPStats4LHC]$ ./Likelihood_syst 10 300 100 10000 .1 .01
------Using the Following Uncertainty------
For Process 0: signal uncertainty = 0.000000
For Process 1: signal uncertainty = 0.000000
For Process 0: background uncertainty = 0.100000
For Process 1: background uncertainty = 0.010000
-----Betup Binning-----
For a single Channel:
                     min log(LR) = 0.029559 max log(LR) = 0.095310
                      totalS = 310.000000
                                             totalB = 10100.000000
Estimating max log(LR) after convolution:
       bin 0: log(LR) = 0.095310, rho_b = 100.000000, rho_sb = 110.000000
       bin 1: log(LR) = 0.029559, rho_b = 10000.000000, rho_sb = 10300.000000
Set Global log(LR): min = 0.000000 max = 598.887708
Need at least 2^13 bins, Perfect binning needs 2^14 bins
Have 2^18 bins, bins for Rho1 = 28.780569
-----Doing FFT's-----
 doing 1000 out of 1000 MC samples, total weight = 1.000000
totalWeight = 1.000000
 doing 1000 out of 1000 MC samples, total weight = 1.000000
totalWeight = 1.000000
Problem Index for Rho_b
                             = -0.000000
                             = -0.000000
Problem Index for Rho_s+b
-----About to Calculate Significance-----
Gaussian Approx: median of rho_b is 68.688123 stdev from hard limit
                Significance is 2.215621
Poisson Approx: mean of rho_b = 124096.379668, stdev = 1806.717004
                Calculated nu = 4717.782983, alpha = 26.303961
                Corresponds to Poisson with b=4717.782983 and s+b=4870.074407
                With No interpolation: median of rho_sb = 4871
                       CL_b = 1.341503e-02, Significance = 2.213981
                With interpolation: median of rho_sb = 4870.074407
                       CL_b = 1.388103e-02, Significance = 2.200632
CL_b integration with no interpolation:
                median of rho_b = 128103, Significance = 2.235173
CL_b integration with interpolation:
                lowerBin = 128102, upperBin = 128103
                beta = 0.247336, generalized median = 128102.247336
                Significance with Interpolation = 2.234740
     -----Summary-----
Sigma(CL_b)
               Sigma(CL_b)(no interp)
                                             Sigma_Gauss
                                                             Sigma_Poisson
                                              2.215621
       Will use integrated CL_b because Gaussian Approx = 2.215621 < 6
Confidence Level is = 2.234740
```